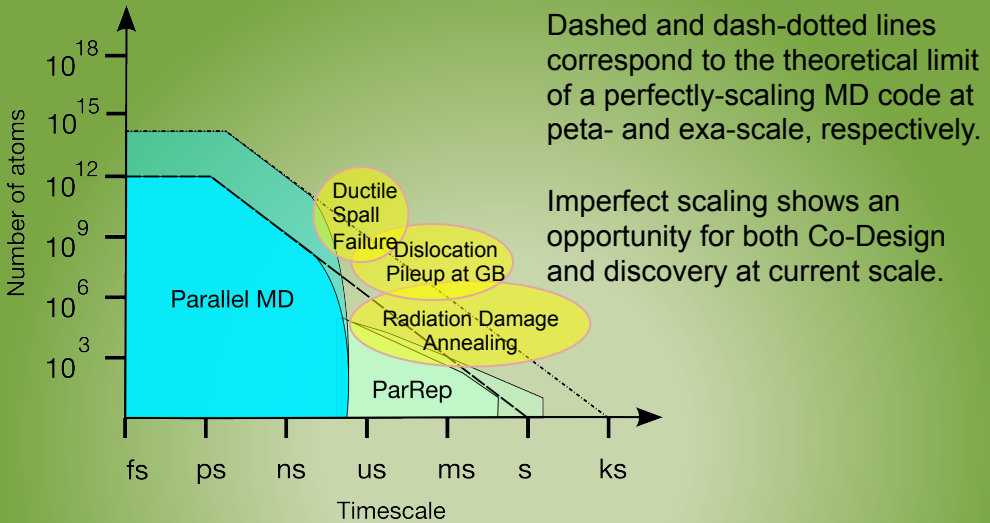# Optimization Principles for Hardware/Software Co-Design
with Applications in Molecular Dynamics

Exascale computing potentially enables the study of new phenomena with MD

Dashed and dash-dotted lines correspond to the theoretical limit of a perfectly-scaling MD code at peta- and exa-scale, respectively.

Imperfect scaling shows an opportunity for both Co-Design and discovery at current scale.

We need new Co-Designed HW architectures and SW algorithms to overcome current and future performance boundaries of MD.

Our approach: cast HW/SW Co-Design problem such that

- Exploration of HW and SW spaces can be automated
- HW/SW pair performance can be predicted
- Finding best HW/SW pair can be posed as a formal optimization problem.

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